Simple and Exact Method for Calculating the Nuclear Reaction Matrix

B. R. Barrett* and R. G. L. Hewitt†
Department of Physics, University of Pittsburgh, Pittsburgh, Pennsylvania ‡ 15213

and

R. J. McCarthy§
Department of Physics, Carnegie-Mellon University, Pittsburgh, Pennsylvania 15213
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A new, simple, and exact method is given for calculating the reaction matrix G in a two-particle harmonic-oscillator basis. The method makes use of an expansion of the Bethe-Goldstone wave function in terms of solutions of the Schrödinger equation for two interacting particles in a harmonic-oscillator well. Since a two-particle basis is used, the Pauli operator Q is diagonal and can be treated exactly. Reaction matrix elements based on the Hamada-Johnston potential are used in a shell-model calculation of $A=18$ nuclei. The results are compared with those of earlier calculations using approximate Pauli operators. The dependence of the reaction matrix on the starting energy is studied, and the relationship of this energy to the intermediate-state spectrum and to the Pauli operator Q is discussed. In this same context the difference between using a Brueckner Q and a shell-model Q is also discussed.

I. INTRODUCTION

We present a simple formalism for calculating reaction matrix elements in a harmonic-oscillator (HO) basis with an exact treatment of the Pauli operator Q. Our approach is based on an earlier suggestion[1] that the Bethe-Goldstone (BG) equation be solved by expanding the BG wave function in terms of eigenfunctions of two *interacting* nucleons bound in the HO well. This suggestion was used previously by Truelove and Nicholls[2] (TN), who developed an interaction scheme for calculating reaction matrix elements based on the integral form of the BG equation. The present method is based on the differential form of the BG equation and the resulting expressions are simpler in form and easier to evaluate numerically.

Our method is related to the reference-spectrum method[3] in that we first calculate a reference matrix G^R and then obtain the reaction matrix G by matrix inversion. The new expression for G^R is, however, quite different from the usual one and allows G^R to be calculated directly in the two-particle representation, where the Pauli operator Q is diagonal.

For the purpose of comparison with earlier calculations, which treated Q only approximately,[4] we perform a simple shell-model calculation for $A=18$ nuclei using G matrix elements calculated with the Hamada-Johnston nucleon-nucleon potential[5] for a wide range of starting energies. We find that an exact treatment of the Pauli operator in the determination of the G matrix can produce sizeable differences in the results obtained for G and for excitation spectra.

In Sec. II we derive our equations for G^R and G, and show that the final expressions are the same for both soft-core and hard-core nucleon-nucleon potentials. Arbitrary shifts in the intermediate-state energies can be made in precisely the same manner as in the usual reference-spectrum method.

In Sec. III we consider separately the calculational procedures for evaluating G^R and G and discuss questions of convergence. We then present the results of an $A=18$ shell-model calculation and compare our results with earlier ones based on an approximate treatment of Q.

Finally, in Sec. IV we discuss the relationship of the starting energy to the intermediate-state spectrum and to the Pauli operator. In this same discussion we point out the difference between using a Brueckner Q and a shell-model Q and show problems which arise in using a shell-model Q.

II. BASIC THEORY

The integral form of the BG equation in a HO basis may be written as

$$\Psi_\alpha^{\mathrm{BG}}(\omega)=\phi_\alpha+\sum_\mu^\infty \frac{Q_\mu \phi_\mu \langle \phi_\mu | V | \Psi_\alpha^{\mathrm{BG}}(\omega)\rangle}{\omega-\epsilon_\mu}\,, \tag{1}$$

where the reaction matrix element $G_{\mu\alpha}(\omega)$ is defined by

$$G_{\mu\alpha}(\omega)=\langle \phi_\mu | V | \Psi_\alpha^{\mathrm{BG}}(\omega)\rangle\,. \tag{2}$$

Here ϕ_μ and ϵ_μ are the eigenstates and eigenvalues of the two-particle HO Hamiltonian H_0; i.e.,

$$H_0\phi_\mu=\epsilon_\mu\phi_\mu\,. \tag{3}$$

[Arbitrary shifts in the two-particle energies of Eq. (1) will be considered later in this section.] The Pauli operator Q, with eigenvalues Q_μ, projects outside the two-particle model space; V is the free nucleon-nucleon potential; and ω is an energy parameter to be determined by the particular application of G.

Our starting point is the differential form of the BG equation. This can be obtained from Eq. (1) by operating on both sides of the equation with $(H_0-\omega)$:

$$(H_0-\omega)\Psi_\alpha^{BG}(\omega)=(\epsilon_\alpha-\omega)\phi_\alpha-\sum_\mu^\infty Q_\mu\phi_\mu G_{\mu\alpha}(\omega)\,. \tag{4}$$

We then use Eq. (2) and the fact that the ϕ_μ form a complete set to rewrite Eq. (4) as

$$(H_0+V-\omega)\Psi_\alpha^{BG}(\omega)=(\epsilon_\alpha-\omega)\phi_\alpha+\sum_\mu^\infty(1-Q_\mu)\phi_\mu G_{\mu\alpha}(\omega)\,. \tag{5}$$

For simplicity we first treat the case where the potential V has no infinite hard core. The form of the left-hand side of Eq. (5) suggests an expansion[1] of $\Psi_\alpha^{BG}(\omega)$ in terms of the complete set of eigenfunctions ψ_i of the Schrödinger equation,

$$(H_0+V)\psi_i=E_i\psi_i \tag{6}$$

for two *interacting* particles bound in the HO well, i.e.,

$$\Psi_\alpha^{BG}(\omega)=\sum_i^\infty a_{i\alpha}(\omega)\psi_i \tag{7}$$

with

$$a_{i\alpha}(\omega)=\langle\psi_i|\Psi_\alpha^{BG}(\omega)\rangle\,. \tag{8}$$

Since the functions ψ_i contain the effects of the strong short-range repulsive part of V, the expansion (7) would be expected to be much more rapidly convergent than the corresponding HO expansion [Eq. (1)]. A simple relation connecting $a_{i\alpha}(\omega)$ with the reaction matrix elements $G_{\mu\alpha}(\omega)$ and the overlaps

$$b_{i\alpha}=\langle\psi_i|\phi_\alpha\rangle \tag{9}$$

can be derived by substituting Eq. (7) into Eq. (5) and making use of Eq. (6) to give

$$\sum_i a_{i\alpha}(\omega)(E_i-\omega)\psi_i=(\epsilon_\alpha-\omega)\phi_\alpha+\sum_\mu(1-Q_\mu)\phi_\mu G_{\mu\alpha}(\omega)\,. \tag{10}$$

Since the functions ψ_i form an orthonormal set, multiplication of both sides of this equation by ψ_i^* and integration over all space yields the desired result:

$$a_{i\alpha}(\omega)=\frac{\epsilon_\alpha-\omega}{E_i-\omega}b_{i\alpha}+\sum_\mu^\infty\frac{1-Q_\mu}{E_i-\omega}b_{i\mu}G_{\mu\alpha}(\omega)\,, \tag{11}$$

whenever ω is not equal to E_i.

The reaction matrix elements can also be expressed in terms of the above quantities.[2,6] If we substitute Eq. (7) into Eq. (2) and then use Eqs. (6), (8), and (9), we find that

$$G_{\beta\alpha}(\omega)=\sum_i^\infty a_{i\alpha}(\omega)b_{i\beta}(E_i-\epsilon_\beta)\,. \tag{12}$$

We may now eliminate $a_{i\alpha}(\omega)$ between Eqs. (11) and (12) to obtain

$$G_{\beta\alpha}(\omega)=(\epsilon_\alpha-\omega)\sum_i^\infty\frac{E_i-\epsilon_\beta}{E_i-\omega}b_{i\alpha}b_i-\sum_i^\infty\sum_\mu^\infty(\epsilon_\mu-\omega)\frac{E_i-\epsilon_\beta}{E_i-\omega}b_{i\beta}b_{i\mu}\left(\frac{1-Q_\mu}{\omega-\epsilon_\mu}\right)G_{\mu\alpha}(\omega) \tag{13}$$

for any ω which is not equal to an eigenvalue of Eq. (6).

If we interchange the order of the infinite sums in the second term on the right-hand side of Eq. (13), the equation can be written in the more transparent form

$$G_{\beta\alpha}(\omega)=G^R_{\beta\alpha}(\omega)-\sum_\mu^\infty G^R_{\beta\mu}(\omega)\frac{1-Q_\mu}{\omega-\epsilon_\mu}G_{\mu\alpha}(\omega)\,, \tag{14}$$

where

$$G^R_{\beta\alpha}(\omega)=(\epsilon_\alpha-\omega)\sum_i^\infty\frac{E_i-\epsilon_\beta}{E_i-\omega}b_{i\alpha}b_{i\beta}\,. \tag{15}$$

It is possible, but tedious, to prove the validity of this interchange by examining the energy dependence of the overlap coefficients $b_{i\alpha}$. However, since interchanging the summation order leads to the standard relationship[3] between the G matrix and the reference matrix G_R, we do not feel that a detailed argument is necessary. It is obvious, however, that the single sum over i in Eq. (15) is absolutely convergent, since the energy-difference ratio is bounded and

$$\sum_i|b_{i\alpha}b_{i\beta}|\leq\tfrac{1}{2}\sum_i(b_{i\alpha}^2+b_{i\beta}^2)=1\,, \tag{16}$$

which follows from the Schwarz inequality. It is also possible to obtain Eq. (15) directly from the reference-spectrum equation

$$(H_0+V-\omega)\Psi^R_\alpha(\omega)=(\epsilon_\alpha-\omega)\phi_\alpha \tag{17}$$

and the definition

$$G^R_{\beta\alpha}(\omega)=\langle\phi_\beta|V|\Psi^R_\alpha(\omega)\rangle\,. \tag{18}$$

The derivation is identical to that given above [Eqs. (6)–(13)], since Eqs. (17) and (18) are the analogs of (5) and (2), respectively.

It is convenient to rewrite our new expression for the reference-spectrum matrix elements in a more elegant form using the orthogonality relation for the HO wave function ϕ_α

$$\sum_i^\infty b_{i\alpha} b_{i\beta} = \delta_{\alpha\beta} . \tag{19}$$

Since the sums over i in both Eqs. (15) and (19) are absolutely convergent, we can rearrange terms to give

$$G^R_{\beta\alpha}(\omega) = (\epsilon_\alpha - \omega)\left[\delta_{\alpha\beta} + \sum_i^\infty \left(\frac{E_i - \epsilon_\beta}{E_i - \omega} - 1 \right) b_{i\alpha} b_{i\beta} \right]$$

$$= (\epsilon_\alpha - \omega)\left[\delta_{\alpha\beta} - (\epsilon_\beta - \omega) \sum_i^\infty \frac{b_{i\alpha} b_{i\beta}}{E_i - \omega} \right] . \tag{20}$$

This last equation displays explicitly the poles and some of the zeros of $G^R_{\beta\alpha}(\omega)$. It is also obvious that $G^R(\omega)$ is Hermitian. Equation (20) is a much more useful form for computational purposes than Eq. (15), since the numerical convergence of the sum over i is significantly improved.

The above treatment can easily be generalized to the case where V contains an infinite repulsive hard core. Here the eigenfunctions ψ_i vanish inside the core and form a complete orthonormal set only for the region outside the core. However, since the BG wave function also vanishes within the core, it may still be expanded in terms of the terms of the ψ_i. It then follows that Eq. (11) for $a_{i\alpha}(\omega)$ remains unchanged. On the other hand, it is necessary to replace Eq. (12) for $G_{\beta\alpha}(\omega)$ by [see Sec. III of Ref. (6)]

$$G_{\beta\alpha}(\omega) = \sum_i^\infty a_{i\alpha}(\omega) b_{i\beta}(E_i - \epsilon_\beta) + (\epsilon_\alpha - \omega) O_{\beta\alpha}$$

$$+ \sum_\mu (1 - Q_\mu) O_{\beta\mu} G_{\mu\alpha}(\omega) . \tag{21}$$

where

$$O_{\beta\alpha} = \int_{|\vec{r}|<c} d\vec{r} \int d\vec{R}\, \phi_\beta^* \phi_\alpha , \tag{22}$$

$\vec{r}$ and $\vec{R}$ are the relative and center-of-mass coordinates of the two particles, and c is the radius of the hard core. Substitution of Eq. (11) into Eq. (21) again yields Eq. (14), provided we change our definition of $G^R_{\beta\alpha}(\omega)$ to

$$G^R_{\beta\alpha}(\omega) = (\epsilon_\alpha - \omega)\left[O_{\beta\alpha} + \sum_i \frac{E_i - \epsilon_\beta}{E_i - \omega} b_{i\alpha} b_{i\beta} \right] . \tag{23}$$

By using the orthogonality relation

$$O_{\beta\alpha} + \sum_i b_{i\alpha} b_{i\beta} = \delta_{\alpha\beta} \tag{24}$$

for the HO wave functions ϕ_α, we again obtain Eq. (20) as our final expression for $G^R_{\beta\alpha}(\omega)$.

We also note that it is possible in this formalism to make arbitrary shifts in the intermediate-state energies in the BG equation, while retaining HO basis functions. The BG equation then becomes

$$\Psi^{BG}_\alpha(\omega) = \phi_\alpha + \sum_\mu^\infty \frac{Q_\mu \phi_\mu G_{\mu\alpha}(\omega)}{\omega - e_\mu} , \tag{25}$$

where we have shifted ϵ_μ to e_μ. If the above derivations are carried through *exactly* as before, the effect is equivalent to making the simple substitution $Q_\mu \to Q'_\mu$ throughout, where

$$Q'_\mu = Q_\mu (\omega - \epsilon_\mu)/(\omega - e_\mu) . \tag{26}$$

Thus our final expression for HO G matrix elements derived from any realistic nucleon-nucleon potential is

$$G_{\beta\alpha}(\omega) = G^R_{\beta\alpha}(\omega)$$

$$- \sum_\mu G^R_{\beta\mu}(\omega) \left(\frac{1}{\omega - \epsilon_\mu} - \frac{Q_\mu}{\omega - e_\mu} \right) G_{\mu\alpha}(\omega) , \tag{27}$$

where

$$G^R_{\beta\alpha}(\omega) = (\epsilon_\alpha - \omega)\left[\delta_{\beta\alpha} - (\epsilon_\beta - \omega) \sum_i^\infty \frac{b_{i\alpha} b_{i\beta}}{E_i - \omega} \right] . \tag{20}$$

III. CALCULATIONS AND RESULTS

A. Calculation of G^R Matrix Elements

The calculation of G^R matrix elements can be conveniently separated into three independent steps. First the eigenvalue equation [Eq. (6)] is solved in the relative coordinate system to obtain a set of relative eigenfunctions $|mS\mathcal{J}T\rangle$ and energies $E_{mS\mathcal{J}T}$. Here S, $\mathcal{J}$, and T are the total spin, angular momentum, and isospin of the eigenfunctions, respectively, while the index m labels eigenfunctions of the same $S\mathcal{J}T$ in order of increasing energy. Some of these eigenfunctions can also be labeled by the orbital angular momentum l. The rest are composed of two wave functions with $l = \mathcal{J} \pm 1$, coupled by the tensor interaction in the nucleon-nucleon potential. In either case we can write

$$|mS\mathcal{J}T\rangle = \sum_l |m(lS)\mathcal{J}T\rangle , \tag{28}$$

where the summation has two terms for coupled waves and only one term for uncoupled waves. Once these eigenfunctions have been obtained, we evaluate the radial overlaps $\langle m(lS)\mathcal{J}T|nl\rangle$, where $|nl\rangle$ represents a relative HO wave function.

The second step consists of evaluating the two-

body overlap coefficients $b_{i\alpha}$. To do this we must discuss the angular momentum coupling of the states ϕ_α and ψ_i. The wave function ϕ_α is the product of two single-particle (SP) HO wave functions coupled to a specific JT:

$$\phi_\alpha \equiv |n_1 l_1 j_1, n_2 l_2 j_2; JT\rangle . \tag{29}$$

The two-body eigenfunction ψ_i is the product of a relative eigenfunction and a HO center-of-mass wave function, again coupled to a total angular momentum J; i.e.,

$$\psi_i \equiv \sum_l |m(lS)\mathcal{J}T, NL; J\rangle . \tag{30}$$

We now express ϕ_α in terms of HO states in the relative-center-of-mass system. Thus

$$\phi_\alpha = \sum{}' C_\alpha[n'l'S'\mathcal{J}'N'L'; JT]\,|n'(l'S')\mathcal{J}'T, N'L'; J\rangle , \tag{31}$$

where the primed summation runs over all primed indices, and the transformation coefficients are given by

$$C_\alpha[nlS\mathcal{J}NL; JT] = \sum_\lambda \frac{[1-(-1)^{S+l+T}]}{[2(1+\delta_{12})]^{1/2}}[(2j_1+1)(2j_2+1)(2\lambda+1)(2S+1)]^{1/2} \begin{Bmatrix} l_1 & l_2 & \lambda \\ \frac{1}{2} & \frac{1}{2} & S \\ j_1 & j_2 & J \end{Bmatrix} \langle nl, NL; \lambda | n_1 l_1, n_2 l_2; \lambda\rangle$$

$$\times (-1)^{S+\lambda+L+\mathcal{J}}[(2\mathcal{J}+1)(2\lambda+1)]^{1/2} \begin{Bmatrix} l & S & \mathcal{J} \\ J & L & \lambda \end{Bmatrix} . \tag{32}$$

In the above equation the symbols enclosed in curly brackets are the usual 9-j and 6-j symbols,[7] respectively; $\langle nl, NL; \lambda | n_1 l_1 n_2 l_2; \lambda\rangle$ is the Brody-Moshinsky transformation bracket,[8] and δ_{12} is equal to unity if the two SP states are identical, and is equal to zero otherwise.

Once the C coefficients have been evaluated, the two-body overlap $b_{i\alpha}$ can be expressed very simply as

$$b_{i\alpha} \equiv \langle \psi_i | \phi_\alpha\rangle = \sum_{n'l'} C_\alpha[n'l'S\mathcal{J}NL; JT]\langle m(l'S)\mathcal{J}T | n'l'\rangle . \tag{33}$$

The summation over l' is restricted to the orbital angular momenta contained in ψ_i, and n' is given by the energy-conservation relation

$$n' = \tfrac{1}{2}(2n_1 + l_1 + 2n_2 + l_2 - 2N - L - l') . \tag{34}$$

We are now in a position to carry out the final step, the summation over i in Eq. (20). The energy E_i is given by

$$E_i = E_{mS\mathcal{J}T} + \epsilon_{NL} , \tag{35}$$

where

$$\epsilon_{NL} = (2N + L + \tfrac{3}{2})\hbar\Omega \tag{36}$$

and $\hbar\Omega$ is the HO spacing. Hence,

$$\sum_i^\infty \frac{b_{i\alpha} b_{i\beta}}{E_i - \omega} = \sum_{S\mathcal{J}NL} \sum_{n'l'} \sum_{n''l''} C_\alpha(n'l'S\mathcal{J}NL; JT) C_\beta(n''l''S\mathcal{J}NL; JT) \sum_m \frac{\langle m(l'S)\mathcal{J}T | n'l'\rangle\langle m(l''S)\mathcal{J}T | n''l''\rangle}{E_{mS\mathcal{J}T} + \epsilon_{NL} - \omega} . \tag{37}$$

All sums, except the one over m, are finite because of the angular momentum and energy-conservation conditions built into the C coefficients. The infinite sum over m must be truncated. As can be seen from the behavior of the radial overlaps shown in Table I, the quantities $b_{i\alpha}$ peak sharply when the energy E_i is approximately equal to the oscillator energy ϵ_α. It is, therefore, obvious from the form of Eq. (37) that the truncation point should be chosen such that E_i is much larger than the three energies ϵ_α, ϵ_β, and ω. In practice we find that matrix elements of G^R are accurate to within 0.02 MeV when E_i is chosen approximately $4\hbar\Omega$ greater than the largest of these three energies. The magnitude of this error is comparable with the numerical uncertainties in evaluating wave functions and radial integrals, which appear in all G-matrix calculations.

One further approximation has been made in carrying out the sum in Eq. (37). Only those eigenstates with relative $\mathcal{J}$ less than or equal to 3 are treated exactly. For all higher partial waves the eigenfunctions are replaced by their corresponding HO wave functions, which means that the eigen-

energies $E_{mS\mathcal{J}T}$ become oscillator energies and the overlaps $\langle m(lS)\mathcal{J}T|\, nl\rangle$ are Kronecker δ functions. This is equivalent to setting the potential V equal to zero for partial waves with $\mathcal{J}>3$.

The above approximation is introduced *only* because the nucleon-nucleon potential is not properly defined in the higher partial waves. Clearly it would be easy to carry out this finite sum exactly if the potential were known. Fortunately, our results *do not depend* on the truncation point provided we include all partial waves with $\mathcal{J}\leq 2$. For heavier nuclei, however, it has been shown[9] that f waves are important, and the truncation point should probably be chosen as $\mathcal{J}=3$ or higher.

B. Calculation of G Matrix Elements

Matrix elements of G can now be obtained from those of G^R using Eq. (27). This equation can be written in matrix form as

$$\begin{pmatrix} A & 0 \\ B & I \end{pmatrix}\begin{pmatrix} G_{\rm I} \\ G_{\rm II} \end{pmatrix}=\begin{pmatrix} G_{\rm I}^R \\ G_{\rm II}^R \end{pmatrix}, \tag{38}$$

where we have ordered the two-particle states α, so that states for which

$$1/(\omega-\epsilon_\alpha)-Q_\alpha/(\omega-e_\alpha)\neq 0 \tag{39}$$

appear first. The matrices A and B are defined by

$$A_{\beta\alpha}=\delta_{\beta\alpha}+G^R_{\beta\alpha}\left(\frac{1}{\omega-\epsilon_\alpha}-\frac{Q_\alpha}{\omega-e_\alpha}\right) \tag{40}$$

and

$$B_{\beta\alpha}=G^R_{\beta\alpha}\left(\frac{1}{\omega-\epsilon_\alpha}-\frac{Q_\alpha}{\omega-e_\alpha}\right). \tag{41}$$

Equation (38) then has the solution

TABLE I. The relative-coordinate S-state overlaps of ψ_1 and ϕ_α for the $^3S_1$-$^3D_1$ state and the $^1S_0$ state. The symbols E_i and E_α here refer to the ***relative*** energy eigenvalues for the state ψ_i and ϕ_α, respectively. Center-of-mass energies are not included. In the $^3S_1$-$^3D_1$ state we have included overlaps only for those states ψ_i which are predominantly S wave. All energies are in MeV.

E_i/E_α	21.0	49.0	77.0	105.0
		$^3S_1$-$^3D_1$		
5.37	0.8862	0.2643	0.1162	0.0518
41.27	−0.3745	0.8876	0.1464	0.0535
71.94	−0.1281	−0.2624	0.9280	0.0972
101.73	−0.0750	−0.1069	−0.1829	0.9479
		$^1S_0$		
13.03	0.9728	0.1756	0.0676	0.0251
44.65	−0.1977	0.9687	0.0931	0.0265
74.69	−0.0632	−0.1224	0.9827	0.0400
104.24	−0.0305	−0.0421	−0.0621	0.9887

$$G_{\rm I}=A^{-1}G_{\rm I}^R, \tag{42}$$

$$G_{\rm II}=G_{\rm II}^R-BG_{\rm I}. \tag{43}$$

Thus, $G_{\rm I}$ and $G_{\rm I}^R$ contain all matrix elements $G_{\beta\alpha}$ and $G^R_{\beta\alpha}$, respectively, for which the state β satisfies the inequality [Eq. (39)]; $G_{\rm II}$ and $G_{\rm II}^R$ contain the remaining matrix elements.

In the present paper we report the results of an $A=18$ shell-model calculation with no independent shifts in the two-particle energies. Thus, in Eqs. (40) and (42) e_α is equal to ϵ_α, and the inequality (39) is satisfied only by those states for which Q_α is equal to zero. These states, which are represented by the shaded area of Fig. 1, consist of all two-particle states for which at least one of the particles is in the $0s$ or $0p$ shells or for which both particles are in the $1s$-$0d$ shell. The infinite set of two-particle states with one particle in the $0s$ or $0p$ shells must be truncated to give a matrix A of finite dimensions.

The effect of this truncation on matrix elements within the s-d shell depends strongly on the energy difference $\omega-\bar{\epsilon}$, where $\bar{\epsilon}$, the maximum two-particle energy retained in the $Q_\mu=0$ space, is determined by the cutoff value of ρ along the wings of Fig. 1. Here $\rho=2n+l$ is the energy quantum number for each major shell within the HO well. In Fig. 2 we show how the lowest 1^+ states of ^{18}F behave as a function of $\rho_{\max}$, for two different values of ω. We find that satisfactory convergence is obtained in all states and for all ω values for a cutoff value of $\rho_{\max}=10$. This cutoff value, which

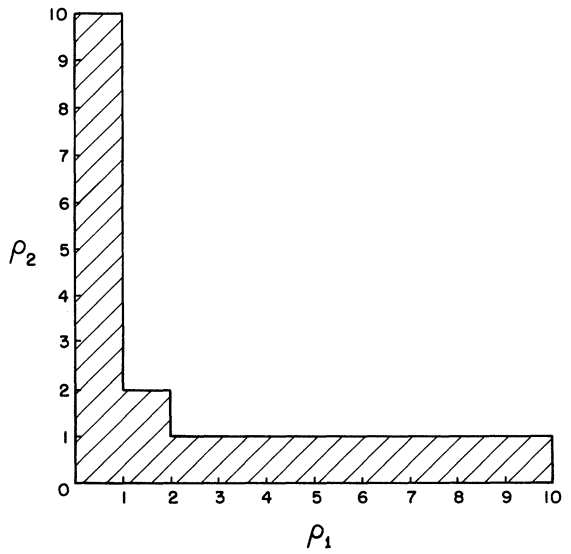

FIG. 1. The shaded area indicates the $Q_\mu=0$ region included in our calculation of the G matrix for $A=18$ nuclei. The symbol $\rho_i=2n_i+l_i$. All appropriate combinations of ρ_1 and ρ_2 within the shaded area determine two-particle configurations used in solving Eq. (42).

leads to dimensions of A varying from 19 by 19 for $J=0$, $T=1$, to 41 by 41 for $J=2$, $T=1$, is used in all our subsequent calculations.

It is, of course, possible to carry out exact calculations of G using G_R matrix elements evaluated by earlier methods. Since the numerical results obtained for G_R here and in Ref. 4 are identical, we should ask which method of calculation is easier and faster. The answer to this question depends somewhat on the size and nature of the calculation but usually the new method is both faster and easier. This is true even though the eigenvalue equation is somewhat more difficult to solve than the relative BG equation.

In the calculations presented here we evaluated 8 relative eigenfunctions for each uncoupled partial wave and 16 for each coupled partial wave up to and including $\mathcal{J}=3$. The total time needed for this calculation – once the codes were working correctly and we could guess good starting values for the eigenvalues – was about four minutes on the Carnegie-Mellon Univac 1108 computer. This calculation never has to be repeated, regardless of the number or range of starting energies used in the BG equation. Moreover, we do not have to worry about calculating G_R for an ω value too close to a pole, since we know the locations of the poles before calculating G_R.

It is faster and easier to calculate individual G_R matrix elements in the relative coordinate system using the older method. However, a large number of these relative matrix elements are needed to obtain each G_R matrix element in the two-body representation. Moreover, we must solve the relative BG equation for a large number of relative starting energies and it is hard to choose these relative starting energies to avoid all singularities in the relative G_R matrix elements. Thus the calculations often have to repeated for new values of the starting energies. As the size of the problem and the range of starting energies increase, the new method presented here becomes more and more advantageous. Of course, a point is reached where time requirements and machine capabilities prevent treating Q exactly, and it becomes best to work entirely in the relative-center-of-mass representation. In this case the new method loses some – but not all – of its advantages.

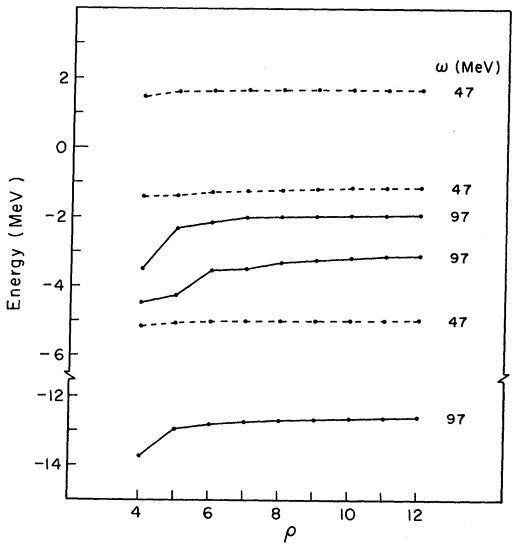

FIG. 2. Convergence of the excitation energies for the three lowest-lying $J^\pi=1^+$, $T=0$ states in ^{18}F, shown as a function of increasing number of major shells (denoted by ρ, see Fig. 1) included in the calculation. Results are given for two values of the energy parameter ω. (Note break in scale for lowest state at $\omega=97$ MeV.)

C. Results

The purpose of this section is to compare our exact treatment of the Pauli operator Q with previous approximate treatments. We therefore study the very simple case of an $A=18$ shell-model calculation without core polarization using the Hamada-Johnston nucleon-nucleon potential[5] and compare our results with those obtained earlier by Mercier, Baranger, and McCarthy,[4] whose results should differ from ours only in the treatment of Q. It would not be meaningful to compare our results directly with those of other investigators[10-13] since the effect of using an exact Q would be masked by other differences in the calculations; e.g., use of different potentials or different intermediate-state spectra.

In Figs. 3 and 4 we plot the excitation energies of ^{18}O and ^{18}F, respectively, as a function of the starting energy ω, and in Fig. 5 we compare our results with those of Mercier *et al.* for the low-lying states of ^{18}F, where the discrepancies are largest. For the purpose of comparison we use the same parameters as Mercier *et al.* [i.e., $\hbar\Omega=14$ MeV and experimental SP energies for ^{17}O ($\epsilon_{0d\,5/2}=0.0$ MeV, $\epsilon_{1s\,1/2}=0.87$ MeV, $\epsilon_{0d\,3/2}=5.08$ MeV)] and present our results for the same range of ω values.

Some of the effects produced by an exact treatment of Q are quite striking. For example, the lowest 2^+ state is strongly depressed by the exact Q at large ω values, causing it to cross below the 5^+ state, an effect not obtained my Mercier *et al.* Although the 1^+ ground state has roughly the same shape in both cases, the exact Q produces an excitation energy which is 1.54 MeV below the approximate Q at $\omega=97$ MeV. In general, the exact Q produces larger differences between the low-lying states than between the higher-lying states.

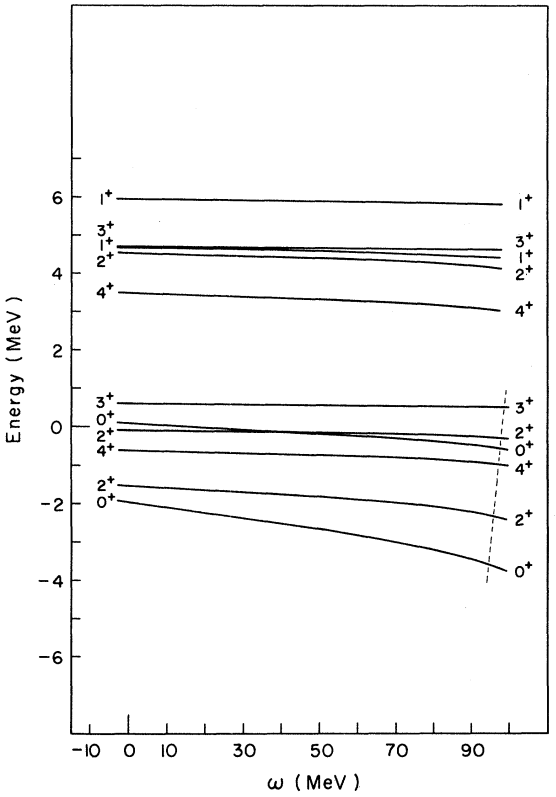

FIG. 3. The low-lying spectra of ^{18}O ($T=1$) as a function of the starting energy ω. The dashed line indicates the self-consistent results for two s-d shell particles in a HO well ($\omega = 98$ MeV$+\Delta E_V$ for $\hbar\Omega = 14$ MeV).

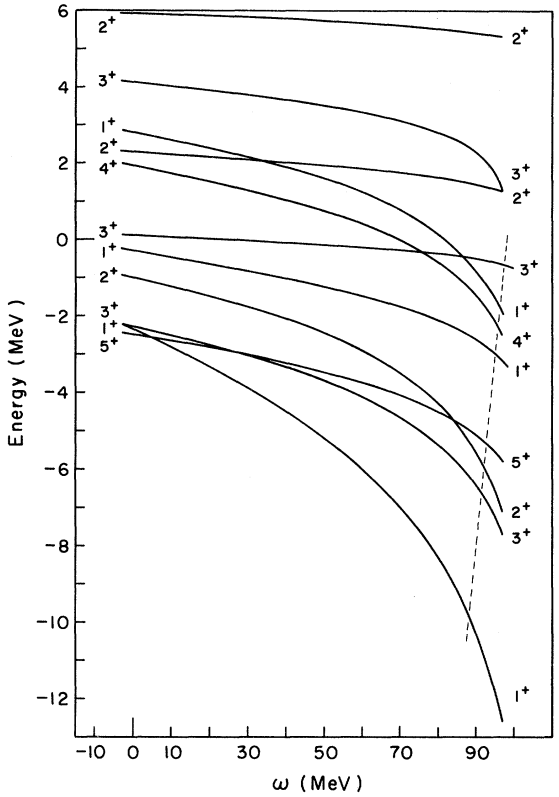

FIG. 4. The low-lying spectra of ^{18}F ($T=0$) as a function of the starting energy ω. The dashed line has the same meaning as in Fig. 3.

The differences at $\omega = -3$ MeV are small in all cases, never being greater than about 0.15 MeV. Both in our results and in those of Mercier *et al.*, all the levels are depressed as the energy parameter ω is increased, since we are approaching the first singularity in the positive-parity G matrix which appears at $\omega \sim 110$ MeV. The differences for the $T=1$ states, which do not contain the strong tensor component of the nucleon-nucleon force, are not as dramatic and range from 0.04 MeV at $\omega = -3$ MeV to 0.28 MeV at $\omega = 97$ MeV for the lowest 0^+ state. In general, the differences at both $\omega = -3$ and 97 MeV are small, being only a few hundredths of an MeV. The first singularity in this case lies higher at $\omega \sim 118$ MeV. It should be noted that all of the discrepancies come entirely from the approximation on Q made by Mercier *et al.*, since their G^R matrix elements are essentially equivalent to ours.

The method of TN[2] also treats the Pauli operator Q exactly and should lead to results identical to ours. Their calculations include a self-consistent determination of the energy parameter ω, and their results should be compared with the points of intersection of the dashed straight lines with the curves in Figs. 3 and 4. We find even larger discrepancies between their results and ours than between those of Mercier *et al.* and ours. Recent studies[14,15] of the TN calculation indicate that they did not include enough terms in their truncated infinite summations.

Finally, it would not be at all meaningful to compare our results with experiment, since second-order[10,11] and higher-order[16] terms in the effective shell-model interaction are known to be important. Consequently, since the effective shell-model interaction is a function of the excitation energy, one must sum the entire perturbation expansion for the effective interaction in order to determine the correct starting value of ω. Thus, even though our G matrices are exact for a given starting energy ω, the precise value of ω to use in evaluating the G matrix elements for performing an effective-interaction shell-model calculation remains uncertain.

In the next section we discuss the physical meaning of the energy parameter ω and its relationship to shifts in the intermediate-state spectrum and to the Pauli operator Q.

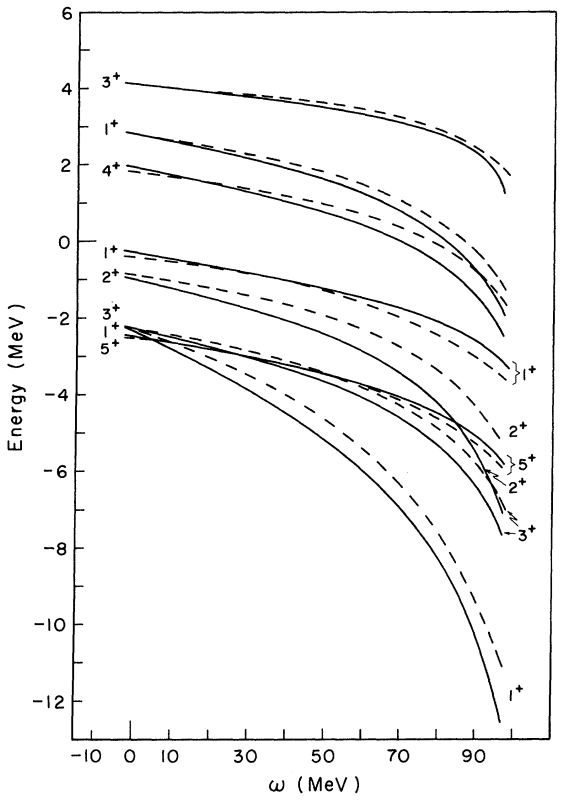

FIG. 5. Comparison of our results for ^{18}F (solid lines) with those of Mercier *et al.* (Ref. 4) (dashed lines) to show the difference produced by an exact and an approximate treatment of the Pauli operator.

IV. DISCUSSION OF TECHNIQUE AND RESULTS

The starting energy ω has been treated so far as a variable parameter which enters the BG equation. In this section we discuss the definition of ω, show how it is related to the choice of the intermediate-state spectrum, and point out some problems which arise when a shell-model Q is used rather than a Brueckner Q.

The starting point for any Brueckner-type calculation – both shell-model and binding energy – is the choice of a SP Hamiltonian to define a set of basis wave functions and energies. The total binding energy or effective interaction is then defined in terms of a perturbation expansion based on these SP wave functions and energies.[17] Obviously, these basis states should be chosen such that the perturbation expansion coverges as rapidly as possible.

Once these basis states are chosen, the value of ω is defined in the Bloch-Horowitz-Brandow theory[17,18] to be the sum of the unperturbed two-particle energy and the self-consistent interaction energy ΔE_V. Two problems arise here. First, the interaction energy ΔE_V is not known until the entire calculation is completed. Thus, we are forced to do the calculation for a range of values of ΔE_V and pick the self-consistent values at the end. A more serious problem is the fact that in calculating only G we are not including enough terms in the Bloch-Horowitz expansion[18] and our results therefore depend upon our original choice of basis states and energies.

In this paper we have chosen the basis states to be defined by HO wave functions. However, it is possible in our formalism to assign independent shifts to each oscillator level and study the resulting spectra as a function of these shifts. The simplest possible type of shift is to introduce a variable energy gap between the occupied and unoccupied SP levels,[19] and it is this type of shift which we wish to discuss.

A gap between occupied and unoccupied SP states can be introduced most simply in binding-energy calculations. Here the G matrix is defined by

$$G_{\alpha\beta}(\omega) = V_{\alpha\beta} + \sum_{\mu} V_{\alpha\mu} \frac{Q_{\mu}^{B}}{\omega - \epsilon_{\mu}} G_{\mu\beta}(\omega) , \tag{44}$$

where Q^B, the Brueckner-Pauli operator, projects only into those two-particle states where *neither* SP state is occupied. Consequently, if we shift the energies of all unoccupied SP states by an amount C, all the ϵ_μ are shifted by an amount $2C$. But this is equivalent to redefining ω as $\omega - 2C$, so it is clear that we can vary the gap between occupied and unoccupied states simply by varying ω.

This simple procedure is not correct in shell-model calculations using a shell-model Q. The shell-model Q projects not only into totally unoccupied two-particle states, but also into those two-particle states in which we have one unoccupied SP state and one valence state. Hence, the use of the nonsymmetrical shell-model Q does not permit the exact separation of valence and unoccupied states simply by varying ω, as in the case of the Brueckner Q.

There are two ways around this difficulty. The first is to continue using a shell-model Q but to extend the matrix-inversion space of Eq. (42) to include those $Q_\mu = 1$ states which contain one valence SP state. Then we can simulate a gap C between occupied and unoccupied SP states by decreasing ω by $2C$ while simultaneously decreasing the energies of the $Q_\mu = 1$ states in the matrix inversion by C. The other method, which also involves increasing the size of the matrix-inversion space, it to use a Brueckner Q in evaluating G. The contribution of SP excitation diagrams to the effective interaction would then have to be evaluated explicitly – again as a function of ω.

In the results presented in Sec. III, the variation with ω cannot be interpreted exactly in terms of a gap between occupied and unoccupied states. We presented our results in that form, however, in order to be able to compare with Mercier *et al.*, who did not treat the shifts exactly. Since a negative shift in ω can always be interpreted as creating a positive gap between the $Q_\mu = 0$ and $Q_\mu = 1$ states, a shell-model Q will introduce too large a gap between the $Q_\mu = 0$ states and the singly occupied $Q_\mu = 1$ states. Thus, for a given shift in ω, our results lie higher than those for a correct treatment of a gap between occupied and unoccupied SP states.

Investigations are presently being carried out by our method to determine the exact effects on the G matrix and on the excitation spectra of nuclei of using a shell-model Q and at the same time properly shifting the intermediate-state spectrum so as to produce a gap between the occupied and unoccupied SP levels. The results of these investigations will be reported in a future publication.

In conclusion we have found that it is important to treat the Pauli operator correctly in shell-model calculations and that further investigations need to be carried out to study the relationship between varying the energy parameter and changing the intermediate-state spectrum. The relationship of these effects to using a shell-model or a Brueckner-Pauli operator also deserves further study.

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*Present address: Department of Physics, University of Arizona, Tucson, Arizona 85721.

†On leave of absence from Department of Physics, University of Sydney, N.S.W. Australia.

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